

ELECTRON WAVEFUNCTIONS AND DENSITIES FOR ATOMS

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ABSTRACT. With a special ‘Ansatz’ we analyse the regularity properties of atomic electron wavefunctions and electron densities. In particular we prove an a priori estimate, $\sup_{y \in B(x, R)} |\nabla \psi(y)| \leq C(R) \sup_{y \in B(x, 2R)} |\psi(y)|$ and obtain for the spherically averaged electron density, $\tilde{\rho}(r)$, that $\tilde{\rho}''(0)$ exists and is non-negative.

Avec un ‘Ansatz’ spécial nous analysons les propriétés de régularité des fonctions d’ondes atomiques et des densités d’électron. En particulier nous prouvons une estimation a priori,

$$\sup_{y \in B(x, R)} |\nabla \psi(y)| \leq C(R) \sup_{y \in B(x, 2R)} |\psi(y)|$$

et obtient pour la densité d’électron moyennée sur la sphère $\tilde{\rho}(r)$, que $\tilde{\rho}''(0)$ existe et est non-négative.

1. INTRODUCTION AND RESULTS

Let V be the Coulomb potential for an atom consisting of a nucleus of charge Z (fixed at the origin) and N electrons:

$$V(\mathbf{x}) = V(x_1, \dots, x_N) = \sum_{j=1}^N -\frac{Z}{|x_j|} + \sum_{1 \leq j < k \leq N} \frac{1}{|x_j - x_k|},$$

$$\mathbf{x} = (x_1, \dots, x_N) \in \mathbb{R}^{3N}, x_j = (x_{j,1}, x_{j,2}, x_{j,3}) \in \mathbb{R}^3, j = 1, \dots, N, \quad (1.1)$$

and let H be the corresponding N -electron Hamilton operator:

$$H \equiv H^N = -\Delta + V \quad (1.2)$$

with

$$-\Delta = \sum_{j=1}^N -\Delta_j \quad , \quad \Delta_j = \sum_{i=1}^3 \frac{\partial^2}{\partial x_{j,i}^2}$$

being the kinetic energy operator of the N electrons. The quadratic form domain of H is $W^{1,2}(\mathbb{R}^{3N})$, see Reed and Simon [12]. Assume

Date: February 1, 2008.

Work supported by Ministerium für Wissenschaft und Verkehr der Republik Österreich, the Austrian Science Foundation, grantnumber P12865-MAT, and by the European Union TMR grant FMRX-CT 96-0001 .

$\psi \in L^2(\mathbb{R}^{3N})$ is a real-valued normalised eigenfunction of the operator H :

$$(H - E)\psi = 0 \quad , \quad \|\psi\| \equiv \|\psi\|_{L^2(\mathbb{R}^{3N})} = 1. \quad (1.3)$$

It is known that then ψ is continuous with bounded derivatives, and $\psi \in W^{2,2}(\mathbb{R}^{3N})$ (Kato [8]) and that ψ is in fact analytic away from the singularities (in \mathbb{R}^{3N}) of V , since V is here real analytic (see Hopf [7]). In this paper we derive various qualitative and quantitative properties of the wave function ψ and of the corresponding one-electron density

$$\rho(x) = \int_{\mathbb{R}^{3(N-1)}} |\psi(x, x_2, \dots, x_N)|^2 dx_2 \dots dx_N \quad , \quad x \in \mathbb{R}^3, \quad (1.4)$$

as well as of its spherical average ($x = r\omega, r = |x|, \omega = x/|x| \in \mathbb{S}^2$)

$$\begin{aligned} \tilde{\rho}(r) &= \int_{\mathbb{S}^2} \rho(r\omega) d\omega \\ &= \int_{\mathbb{S}^2} \int_{\mathbb{R}^{3(N-1)}} |\psi(r\omega, x_2, \dots, x_N)|^2 dx_2 \dots dx_N d\omega \quad , \quad r \in [0, \infty). \end{aligned} \quad (1.5)$$

Remark 1.1. Aside from Kato's classical results (see Kato [8]), the local behaviour of electron wavefunctions has been investigated more recently by Hoffmann-Ostenhof et al. [4], [6]. The electron density itself has been studied extensively in the large- Z -limit, see Lieb [9]. Except for the spatial asymptotics, see Ahlrichs et al. [1], there are virtually no recent rigorous results on ρ despite the fact that the density is the central object in various popular numerical approximation schemes, as Density Functional Theory (DFT) and all the various descendants of Hartree-Fock theory.

We now present our results.

Theorem 1.2. *Let ψ be as in (1.3). For all $R \in (0, \infty)$, there exists a constant $C = C(R)$ such that*

$$\sup_{\mathbf{y} \in B(\mathbf{x}, R)} |\nabla \psi(\mathbf{y})| \leq C \sup_{\mathbf{y} \in B(\mathbf{x}, 2R)} |\psi(\mathbf{y})| \quad \text{for all } \mathbf{x} \in \mathbb{R}^{3N}.$$

Remark 1.3. This result complements the result by Simon [14, Thm. C.2.5 (C14)] for the case of operators of the form (1.2), but with V in the Kato-class $K^{n,1}(\mathbb{R}^n)$: for $\delta \in [0, 2)$ ($\delta = 0 : n \geq 3$),

$$V \in K^{n,\delta}(\mathbb{R}^n) \Leftrightarrow \limsup_{\epsilon \rightarrow 0} \sup_{x \in \mathbb{R}^n} \int_{|x-y|<\epsilon} \frac{|V(y)|}{|x-y|^{n-2+\delta}} dy = 0.$$

The Coulomb potential (1.1) is in $K^{3N,\delta}(\mathbb{R}^{3N})$ for all $\delta \in [0, 1)$, but is not in $K^{3N,1}(\mathbb{R}^{3N})$.

We recall the definition of Hölder continuity:

Definition 1.4. For $\Omega \subset \mathbb{R}^n$ an open set, $k \in \mathbb{N}$, and $\alpha \in (0, 1]$, we say that the function u belongs to $C_{\text{loc}}^{k,\alpha}(\Omega)$ whenever $u \in C^k(\Omega)$, and for all $\beta \in \mathbb{N}^n$ with $|\beta| = k$, and all open balls $B(x_0, r) \subset \Omega$, we have

$$\sup_{x,y \in B(x_0, r), x \neq y} \frac{|D^\beta u(x) - D^\beta u(y)|}{|x - y|^\alpha} \leq C(x_0, r).$$

As a consequence of the proof of Theorem 1.2 we get:

Proposition 1.5. *Let*

$$F(\mathbf{x}) = F(x_1, \dots, x_N) = \sum_{j=1}^N -\frac{Z}{2}|x_j| + \sum_{1 \leq j < k \leq N} \frac{1}{4}|x_j - x_k|. \quad (1.6)$$

Then the eigenfunction ψ given in (1.3) can be represented as

$$\psi = e^F \phi$$

with

$$\phi \in C_{\text{loc}}^{1,\alpha}(\mathbb{R}^{3N}) \text{ for all } \alpha \in (0, 1).$$

Remark 1.6. This result classifies the singularities of $\nabla\psi$ as those coming from ∇F : $\nabla\psi = \psi\nabla F + e^F\nabla\phi$. Kato [8] proved that $\nabla\psi$ is bounded, but as the ground state of Hydrogen-like systems ($N = 1, E = -Z^2/4$, $\psi(x) = c_0 e^{-Z|x|/2}, x \in \mathbb{R}^3$) shows, it is not in general continuous.

Remark 1.7. The results of Theorem 1.2 and Proposition 1.5 easily generalise to the case of molecules: L nuclei, of charge Z_l , fixed at $R_l \in \mathbb{R}^3$, $l = 1, \dots, L$, with corresponding N -electron Hamilton operator

$$H^{N,L} = \sum_{j=1}^N \left(-\Delta_j - \sum_{l=1}^L \frac{Z_l}{|x_j - R_l|} \right) + \sum_{1 \leq j < k \leq N} \frac{1}{|x_j - x_k|}.$$

We assume throughout when studying ρ and $\tilde{\rho}$ that E and ψ in (1.3) are such that there exist constants $C_0, \gamma > 0$ such that

$$|\psi(\mathbf{x})| \leq C_0 e^{-\gamma|\mathbf{x}|} \text{ for all } \mathbf{x} \in \mathbb{R}^{3N}. \quad (1.7)$$

For references on the exponential decay of eigenfunctions, see e. g. Simon [14].

Remark 1.8. Inequality (1.7) holds when $E < \inf \sigma_{\text{ess}}(H^N)$. In this case, we let $\varepsilon \equiv E_0^{N-1} - E$ with E_0^{N-1} the ground state energy of the $(N-1)$ -electron operator:

$$H^{N-1} = \sum_{j=2}^N \left(-\Delta_j - \frac{Z}{|x_j|} \right) + \sum_{2 \leq j < k \leq N} \frac{1}{|x_j - x_k|}. \quad (1.8)$$

By the HVZ-theorem (see Cycon et al. [2, Theorem 3.7], $\inf \sigma_{\text{ess}}(H^N) = E_0^{N-1}$, and so $\varepsilon > 0$ if $E < \inf \sigma_{\text{ess}}(H^N)$). When we study H in a symmetry sector, so that ψ transforms according to this symmetry, then E_0^{N-1} stands for the groundstate energy of the ionized particle system described by the Hamiltonian H^{N-1} in the appropriate symmetry subspace as determined by the symmetry behaviour of ψ . For this case a modified version of the HVZ-theorem holds (see e. g. Reed and Simon [13, Thm. XIII. 17] and Zhislin and Sigalov [15]). This includes in particular the physically important case of real atoms (Pauli principle). So if E lies below the beginning of the essential spectrum of H considered in a symmetry sector, then analogously to the above the ionisation energy $\varepsilon > 0$ and ψ satisfies (1.7).

Remark 1.9. When assuming (1.7), Theorem 1.2 implies that $|\nabla \psi(\mathbf{x})|$ also decays exponentially for $|\mathbf{x}| \rightarrow \infty$.

Remark 1.10. From (1.7) and Lebesgue's Dominated Convergence Theorem follows that the density ρ is continuous in \mathbb{R}^3 .

Theorem 1.11. *Let ψ be given according to (1.3) and assume that (1.7) holds. Then:*

- (i) *The function ρ defined in (1.4) satisfies, in the distributional sense, the equation*

$$-\frac{1}{2}\Delta\rho - \frac{Z}{r}\rho + h = 0 \quad \text{in } \mathbb{R}^3, \quad (1.9)$$

where

$$h \in C^\alpha(\mathbb{R}^3 \setminus \{0\}) \cap L^\infty(\mathbb{R}^3) \quad \text{for all } \alpha \in (0, 1)$$

and

$$\rho \in C^{2,\alpha}(\mathbb{R}^3 \setminus \{0\}) \cap C^{0,1}(\mathbb{R}^3) \quad \text{for all } \alpha \in (0, 1).$$

- (ii) *The function $\tilde{\rho}$ defined in (1.5) satisfies*

$$-\frac{1}{2}\Delta\tilde{\rho} - \frac{Z}{r}\tilde{\rho} + \tilde{h} = 0 \quad \text{for } r > 0 \quad (1.10)$$

where $\tilde{h}(r) = \int_{\mathbb{S}^2} h(r\omega) d\omega$. Thereby,

$$\tilde{h} \in C^\alpha((0, \infty)) \cap C^0([0, \infty)) \quad \text{for all } \alpha \in (0, 1)$$

and

$$\tilde{\rho} \in C^{2,\alpha}((0, \infty)) \cap C^2([0, \infty)) \quad \text{for all } \alpha \in (0, 1).$$

(iii)

$$h(x) \leq C(R) \left(\int_{B(x,R)} \rho(y) dy + \rho(x) \right) \quad \text{for all } x \in \mathbb{R}^3, \quad (1.11)$$

$$h(x) \geq \varepsilon \rho(x) \quad \text{for all } x \in \mathbb{R}^3, \quad \text{if } \varepsilon = E_0^{N-1} - E > 0. \quad (1.12)$$

(iv)

$$\left(\frac{d^2}{dr^2} \tilde{\rho} \right)(0) = \frac{2}{3} (\tilde{h}(0) + Z^2 \tilde{\rho}(0)). \quad (1.13)$$

Remark 1.12. The results in (i) generalize to the case of molecules, where the continuity results for ρ and h hold in the complement of the set $\{R_1, \dots, R_L\} \subset \mathbb{R}^3$ (see Remark 1.7).

Remark 1.13. It is known that eigenfunctions obey (Kato's) Cusp Condition (see Kato [8]), and similar properties hold for particle densities. For more recent results see Hoffmann-Ostenhof et al. [4], [5], Hoffmann-Ostenhof and Seiler [6]. In the proof of Theorem 1.11, (iv) we make use of the Cusp Condition for $\tilde{\rho}$, namely:

$$\tilde{\rho}'(0) = \lim_{r \downarrow 0} \frac{\tilde{\rho}(r) - \tilde{\rho}(0)}{r} = -Z\tilde{\rho}(0) \quad \text{and} \quad \lim_{r \downarrow 0} \tilde{\rho}'(r) = \tilde{\rho}'(0) \quad (1.14)$$

and also present a proof for it.

Remark 1.14. Of course our results are only first steps in a thorough investigation of qualitative properties of the one-electron density. Here are some obvious open questions:

- (i) Is $\rho(x) > 0$ for all $x \in \mathbb{R}^3$? We remark that this cannot be true in general, since it is false for some excited states of Hydrogen.
- (ii) Is $\rho \in C^\infty(\mathbb{R}^3 \setminus \{0\})$ or even $C^\omega(\mathbb{R}^3 \setminus \{0\})$?
- (iii) Is $\tilde{\rho}$ smooth in $[0, \infty)$, in the sense that $(\frac{d^k}{dr^k} \tilde{\rho})(r)$ exists for $r \geq 0$ for all k ?
- (iv) Is $\frac{d}{dr} \tilde{\rho}(r) \leq 0$ for $r \geq 0$? This is expected to be true for groundstate densities, but not known even for the bosonic case like Helium. Our results imply that $\frac{d}{dr} \tilde{\rho}(r) \leq 0$ for $r \leq R_0$ for the bosonic case, where R_0 depends on the constant C in Theorem 1.2. Note that because of (1.9) and (1.12) we have $\Delta \rho \geq 0$ for $|x| \geq Z/\varepsilon$, and so the Maximum Principle gives that $\frac{d}{dr} \tilde{\rho}(r) < 0$ for $r > Z/\varepsilon$.

Remark 1.15. In the proof of Theorem 1.11 we obtain (see Proposition 3.1): With $\nabla_1 = (\frac{\partial}{\partial x_{1,1}}, \frac{\partial}{\partial x_{1,2}}, \frac{\partial}{\partial x_{1,3}})$, the function

$$t_1(r) = \int_{\mathbb{S}^2} \int_{\mathbb{R}^{3(N-1)}} |\nabla_1 \psi(r\omega, x_2, \dots, x_N)|^2 dx_2 \dots dx_N d\omega$$

is continuous on $[0, \infty)$.

2. PROOFS

Throughout the proofs, we will denote by C generic constants.

Crucial for our investigations is Corollary 8.36 in Gilbarg and Trudinger [3]. We shall make use of this result several times and for convenience we state it already here, adapted for our special case:

Proposition 2.1. *Let Ω be a bounded domain in \mathbb{R}^n and suppose $u \in W^{1,2}(\Omega)$ is a weak solution of $\Delta u + \sum_{j=1}^n b_j D_j u + Wu = g$ in Ω , where $b_j, W, g \in L^\infty(\Omega)$. Then $u \in C^{1,\alpha}(\Omega)$ for all $\alpha \in (0, 1)$ and for any domain Ω' , $\overline{\Omega'} \subset \Omega$ we have*

$$|u|_{C^{1,\alpha}(\Omega')} \leq C \left(\sup_{\Omega} |u| + \sup_{\Omega} |g| \right)$$

for $C = C(n, M, \text{dist}(\Omega', \partial\Omega))$, with

$$\max_{j=1,\dots,n} \{1, \|b_j\|_{L^\infty(\Omega)}, \|W\|_{L^\infty(\Omega)}, \|g\|_{L^\infty(\Omega)}\} \leq M.$$

Thereby

$$|u|_{C^{1,\alpha}(\Omega')} = \|u\|_{L^\infty(\Omega')} + \|\nabla u\|_{L^\infty(\Omega')} + \sup_{x,y \in \Omega', x \neq y} \frac{|\nabla u(x) - \nabla u(y)|}{|x - y|^\alpha}.$$

Proof of Theorem 1.2 and Proposition 1.5.

Let the function F be as in (1.6) and define the function F_1 by

$$F_1(x_1, \dots, x_N) = \sum_{j=1}^N -\frac{Z}{2} \sqrt{|x_j|^2 + 1} + \sum_{1 \leq j < k \leq N} \frac{1}{4} \sqrt{|x_j - x_k|^2 + 1}. \quad (2.1)$$

A computation shows that

$$\Delta F = V, \quad (2.2)$$

$$\begin{aligned} \|F - F_1\|_{L^\infty(\mathbb{R}^{3N})}, \quad & \|\nabla(F - F_1)\|_{L^\infty(\mathbb{R}^{3N})}, \quad \|D^\beta F_1\|_{L^\infty(\mathbb{R}^{3N})} \\ & \leq C(\beta, N, Z), \quad |\beta| \geq 1. \end{aligned} \quad (2.3)$$

Make the ‘Ansatz’ $\psi = e^{F-F_1}\psi_1$. Using $(H - E)\psi = 0$ and (2.2) we get that ψ_1 satisfies the equation

$$\Delta\psi_1 + 2\nabla(F - F_1) \cdot \nabla\psi_1 + (|\nabla(F - F_1)|^2 - \Delta F_1 + E)\psi_1 = 0. \quad (2.4)$$

Due to (2.3) the coefficients in (2.4) are bounded in \mathbb{R}^{3N} . Then Proposition 2.1 implies that ψ_1 is $C^{1,\alpha}$ for all $\alpha \in (0, 1)$, in any ball $B(\mathbf{x}, R) \subset \mathbb{R}^{3N}$, and

$$|\psi_1|_{C^{1,\alpha}(B(\mathbf{x}, R))} \leq C \sup_{y \in B(\mathbf{x}, 2R)} |\psi_1(y)| \quad (2.5)$$

with C depending on R but not on \mathbf{x} . Since

$$|\nabla\psi(\mathbf{y})| \leq |\nabla(F - F_1)| |\psi(\mathbf{y})| + |e^{F-F_1} \nabla\psi_1(\mathbf{y})|$$

we obtain, via (2.3) and (2.5),

$$\begin{aligned} \sup_{\mathbf{y} \in B(\mathbf{x}, R)} |\nabla \psi(\mathbf{y})| &\leq C \left(\sup_{\mathbf{y} \in B(\mathbf{x}, R)} |\psi(\mathbf{y})| + \sup_{\mathbf{y} \in B(\mathbf{x}, R)} |\nabla \psi_1(\mathbf{y})| \right) \\ &\leq C \left(\sup_{\mathbf{y} \in B(\mathbf{x}, 2R)} |\psi(\mathbf{y})| + \sup_{\mathbf{y} \in B(\mathbf{x}, 2R)} |\psi_1(\mathbf{y})| \right) \leq C \sup_{\mathbf{y} \in B(\mathbf{x}, 2R)} |\psi(\mathbf{y})|, \end{aligned}$$

with $C = C(R)$. This proves Theorem 1.2.

Proposition 1.5 follows from $\psi = e^{F-F_1}\psi_1$, $\psi_1 \in C_{\text{loc}}^{1,\alpha}(B(\mathbf{x}, R))$, since e^{-F_1} is smooth. \square

Proof of Theorem 1.11.

Multiplying the equation $(H - E)\psi = 0$ with ψ and integrating over x_2, \dots, x_N gives the equation

$$\begin{aligned} \int_{\mathbb{R}^{3(N-1)}} \psi \Delta_1 \psi \, dx_2 \cdots dx_N + \frac{Z}{|x_1|} \rho(x_1) &= \\ &= \sum_{j=2}^N \int_{\mathbb{R}^{3(N-1)}} \psi \left(-\Delta_j - \frac{Z}{|x_j|} \right) \psi \, dx_2 \cdots dx_N \\ &\quad + \sum_{1 \leq j < k \leq N} \int_{\mathbb{R}^{3(N-1)}} \frac{1}{|x_j - x_k|} \psi^2 \, dx_2 \cdots dx_N \\ &= \int_{\mathbb{R}^{3(N-1)}} \psi (H^{N-1} - E) \psi \, dx_2 \cdots dx_N \\ &\quad + \sum_{j=2}^N \int_{\mathbb{R}^{3(N-1)}} \frac{1}{|x_1 - x_j|} \psi^2 \, dx_2 \cdots dx_N \end{aligned} \tag{2.6}$$

where H^{N-1} is the $(N-1)$ -electron operator defined in (1.8). Since $\Delta_1(\psi^2) = 2|\nabla_1 \psi|^2 + 2\psi \Delta_1 \psi$ and $\int \Delta_1(\psi^2)(x_1, x') \, dx' = \Delta_1 \rho$ in the distributional sense, we get that

$$\begin{aligned} \frac{1}{2} \Delta_1 \rho(x_1) &= \int_{\mathbb{R}^{3(N-1)}} |\nabla_1 \psi|^2 \, dx_2 \cdots dx_N \\ &\quad + \int_{\mathbb{R}^{3(N-1)}} \psi \Delta_1 \psi \, dx_2 \cdots dx_N \end{aligned} \tag{2.7}$$

which, together with (2.6), gives the equation ($r = |x|$)

$$\begin{aligned} \frac{1}{2} \Delta \rho(x) + \frac{Z}{r} \rho(x) &= \int_{\mathbb{R}^{3(N-1)}} \psi (H^{N-1} - E) \psi \, dx_2 \cdots dx_N \\ &\quad + \sum_{j=2}^N \int_{\mathbb{R}^{3(N-1)}} \frac{1}{|x_1 - x_j|} \psi^2 \, dx_2 \cdots dx_N \\ &\quad + \int_{\mathbb{R}^{3(N-1)}} |\nabla_1 \psi|^2 \, dx_2 \cdots dx_N \equiv h(x), \end{aligned} \tag{2.8}$$

hence we obtain (1.9). Integration of (1.9) over \mathbb{S}^2 yields (1.10).

The proof of the regularity properties of the functions h and \tilde{h} are rather technical, and therefore postponed to the next section.

We now verify the regularity properties of the functions ρ and $\tilde{\rho}$ under the assumption that the regularity properties of h and \tilde{h} stated in Theorem 1.11 have been shown. Define the function μ by the equation ($r = |x|$)

$$\rho(x) = e^{-Zr}(\rho(0) + \mu(x)). \quad (2.9)$$

Then $\mu = e^{Zr}\rho - \rho(0)$, $\mu(0) = 0$, and (2.8) implies that

$$\Delta\mu - 2Z\frac{x}{r} \cdot \nabla\mu + Z^2\mu = 2he^{Zr} - Z^2\rho(0). \quad (2.10)$$

Since $h \in L_{\text{loc}}^\infty$, all coefficients of (2.10) are L_{loc}^∞ , and since $\rho \in W_{\text{loc}}^{1,2}$, also $\mu \in W_{\text{loc}}^{1,2}$. Therefore Proposition 2.1 leads to $\mu \in C_{\text{loc}}^{1,\alpha}$, for all $\alpha \in (0, 1)$. Due to (2.9), $\rho \in C^{0,1}(\mathbb{R}^3)$ follows.

Now consider

$$\Delta\rho = -\frac{2Z}{r}\rho + 2h \equiv g \quad \text{in } \mathbb{R}^3 \setminus \{0\}. \quad (2.11)$$

Since $h \in C^\alpha(\mathbb{R}^3 \setminus \{0\})$, for all $\alpha \in (0, 1)$ and due to the above, $\rho/r \in C^\alpha(\mathbb{R}^3 \setminus \{0\})$, for all $\alpha \in (0, 1)$, we have

$$g \in C^\alpha(\mathbb{R}^3 \setminus \{0\}) \text{ for all } \alpha \in (0, 1). \quad (2.12)$$

From (2.11) and (2.12) we obtain from regularity theory for the Poisson equation that $\rho \in C^{2,\alpha}(\mathbb{R}^3 \setminus \{0\})$ (see e. g. Gilbarg and Trudinger [3, Thm. 4.3 and 4.6] or Lieb and Loss [10, Thm. 10.3]).

We proceed analogously for $\tilde{\rho}$: integrating (2.11) over \mathbb{S}^2 , we get the equation

$$\Delta\tilde{\rho} = -\frac{2Z}{r}\tilde{\rho} + 2\tilde{h} \equiv \tilde{g} \quad \text{in } \mathbb{R}^3 \setminus \{0\} \quad (2.13)$$

with

$$\tilde{h}(r) = \int_{\mathbb{S}^2} h(r\omega) d\omega. \quad (2.14)$$

Since the R.H.S. of (2.13) is in $C^\alpha(\mathbb{R}^3 \setminus \{0\})$, we obtain that $\tilde{\rho}$ as a (radially symmetric) function in \mathbb{R}^3 is $C^{2,\alpha}$ away from the origin, and therefore $\tilde{\rho} : \mathbb{R}_+ \rightarrow \mathbb{R}$ satisfies $\tilde{\rho} \in C^{2,\alpha}((0, \infty))$.

That $\tilde{\rho} \in C^2([0, \infty))$ is shown in the proof of (iv).

Next we prove (iii). To prove the bound (1.12), let E_0^{N-1} be the groundstate energy for the operator H^{N-1} . From Remark 1.8 and the Variational Principle we get that for almost all $x_1 \in \mathbb{R}^3$,

$$\int_{\mathbb{R}^{3(N-1)}} \psi(H^{N-1} - E)\psi dx_2 \cdots dx_N \geq (E_0^{N-1} - E)\rho(x_1),$$

and so $h(x) \geq \varepsilon \rho(x)$ with $\varepsilon = E_0^{N-1} - E > 0$.

As for the bound (1.11), note that due to the operator inequality $-\Delta - \beta/r \geq -\beta^2/4$ (true in dimension 3) and the translation invariance of $-\Delta$ we have, for almost all $x_k \in \mathbb{R}^3$ (fixed), $k \in \{1, \dots, N\}$, $k \neq j$,

$$\int_{\mathbb{R}^3} \frac{1}{|x_j - x_k|} |\psi|^2 dx_j \leq \int_{\mathbb{R}^3} |\nabla_j \psi|^2 dx_j + \frac{1}{4} \int_{\mathbb{R}^3} |\psi|^2 dx_j.$$

In this way, using (2.7),

$$h(x) \leq C \left(\int_{\mathbb{R}^{3(N-1)}} |\nabla \psi|^2 dx_2 \cdots dx_N + \int_{\mathbb{R}^{3(N-1)}} |\psi|^2 dx_2 \cdots dx_N \right). \quad (2.15)$$

Due to Theorem 1.2 and a subsolution estimate (see Simon [14, Theorem C.1.2.]) we get, with $\mathbf{x} = (x_1, \dots, x_N) = (x_1, x')$, $x' \in \mathbb{R}^{3(N-1)}$ and χ_Ω the characteristic function of the set Ω :

$$\begin{aligned} |\nabla \psi(\mathbf{x})|^2 &\leq C \sup_{\mathbf{y} \in B(\mathbf{x}, R)} |\psi(\mathbf{y})|^2 \leq C \int_{\mathbf{y} \in B(\mathbf{x}, 2R)} |\psi(\mathbf{y})|^2 d\mathbf{y} \\ &= C \int_{\mathbb{R}^{3N}} \chi_{B(\mathbf{x}, 2R)}(\mathbf{y}) |\psi(\mathbf{y})|^2 d\mathbf{y}. \end{aligned}$$

Using this, and that for fixed $\mathbf{x}, \mathbf{y} \in \mathbb{R}^{3N}$:

$$\chi_{B(\mathbf{x}, 2R)}(\mathbf{y}) = \chi_{B(\mathbf{y}, 2R)}(\mathbf{x}) = \begin{cases} 1 & \text{if } |\mathbf{x} - \mathbf{y}| < 2R, \\ 0 & \text{otherwise} \end{cases}$$

we get, by Fubini,

$$\begin{aligned} &\int_{\mathbb{R}^{3(N-1)}} |\nabla \psi(x_1, x')|^2 dx' \\ &\leq C \int_{\mathbb{R}^{3(N-1)}} \left(\int_{\mathbb{R}^{3N}} \chi_{B(\mathbf{x}, 2R)}(\mathbf{y}) |\psi(\mathbf{y})|^2 d\mathbf{y} \right) dx' \\ &= C \int_{\mathbb{R}^{3N}} |\psi(\mathbf{y})|^2 \left(\int_{\mathbb{R}^{3(N-1)}} \chi_{B(\mathbf{y}, 2R)}(\mathbf{x}) dx' \right) d\mathbf{y}. \end{aligned} \quad (2.16)$$

Note that with $\mathbf{z} = \mathbf{x} - \mathbf{y}$ we have

$$\chi_{B(\mathbf{y}, 2R)}(\mathbf{x}) = \chi_{B(\mathbf{y}, 2R)}(\mathbf{z} + \mathbf{y}) = \chi_{B(\mathbf{0}, 2R)}(\mathbf{z})$$

and so (with $r' = |z'|$ and $\omega' = z'/r'$)

$$\begin{aligned} \int_{\mathbb{R}^{3(N-1)}} \chi_{B(\mathbf{y}, 2R)}((x_1, x')) dx' &= \int_{\mathbb{R}^{3(N-1)}} \chi_{B(\mathbf{0}, 2R)}((z_1, z')) dz' \\ &= \int_{|(z_1, z')| \leq 2R} dz' = \chi_{B(0, 2R)}(z_1) \int_{\mathbb{S}^{3(N-1)-1}} \int_0^{\sqrt{4R^2 - |z_1|^2}} r'^{3(N-1)-1} dr' d\omega' \\ &= C(N) (4R^2 - |z_1|^2)^{3(N-1)/2} \chi_{B(0, 2R)}(z_1) \\ &\leq \tilde{C}(N) R^{3(N-1)} \chi_{B(x_1, 2R)}(y_1). \end{aligned} \quad (2.17)$$

From (2.16) and (2.17) we get

$$\begin{aligned} & \int_{\mathbb{R}^{3(N-1)}} |\nabla \psi(x_1, x')|^2 dx' \\ & \leq C(R) \int_{|x_1 - y_1| < 2R} \int_{\mathbb{R}^{3(N-1)}} |\psi(y_1, y')|^2 dy' dy_1 = C(R) \int_{B(x_1, 2R)} \rho(y_1) dy_1. \end{aligned} \quad (2.18)$$

Combining (2.15) and (2.18) proves (1.11).

We now prove (iv). We first prove Kato's Cusp Condition (1.14) for the function $\tilde{\rho}$:

$$\tilde{\rho}'(0) = \lim_{r \downarrow 0} \frac{\tilde{\rho}(r) - \tilde{\rho}(0)}{r} = -Z\tilde{\rho}(0) \text{ and } \lim_{r \downarrow 0} \tilde{\rho}'(r) = \tilde{\rho}'(0).$$

First, define the function $\tilde{\mu}$ by the equation (see also (2.9))

$$\tilde{\rho}(r) = e^{-Zr}(\tilde{\rho}(0) + \tilde{\mu}(r)). \quad (2.19)$$

Note that $\tilde{\mu}(0) = 0$. Then, using (1.10), $\tilde{\mu}$ satisfies the equation

$$\Delta \tilde{\mu} - 2Z \frac{x}{r} \cdot \nabla \tilde{\mu} + Z^2 \tilde{\mu} = 2\tilde{h}e^{Zr} - Z^2 \tilde{\rho}(0),$$

and, since \tilde{h} is continuous, Proposition 2.1 gives that $\tilde{\mu}$, as a (radially symmetric) function in \mathbb{R}^3 , is $C^{1,\alpha}$ in a neighbourhood of the origin. In particular, $\lim_{r \downarrow 0} \tilde{\mu}'(r) = \tilde{\mu}'(0)$. Since (see (2.19))

$$\tilde{\rho}'(r) = -Z\tilde{\rho}(0) + e^{-Zr}\tilde{\mu}'(r) \quad (2.20)$$

this means that

$$\lim_{r \downarrow 0} \tilde{\rho}'(r) = -Z\tilde{\rho}(0) + \lim_{r \downarrow 0} \tilde{\mu}'(r) = \tilde{\mu}'(0) - Z\tilde{\rho}(0). \quad (2.21)$$

From (2.19) we also get that

$$\frac{\tilde{\mu}(r)}{r} = e^{Zr} \frac{\tilde{\rho}(r) - \tilde{\rho}(0)}{r} + \frac{e^{Zr} - 1}{r} \tilde{\rho}(0).$$

This, together with (2.21) and $\tilde{\mu}(0) = 0$, implies that

$$\begin{aligned} \lim_{r \downarrow 0} \tilde{\rho}'(r) &= \tilde{\mu}'(0) - Z\tilde{\rho}(0) = \lim_{r \downarrow 0} \frac{\tilde{\mu}(r)}{r} - \tilde{\rho}(0) \lim_{r \downarrow 0} \frac{e^{Zr} - 1}{r} \\ &= \lim_{r \downarrow 0} e^{Zr} \frac{\tilde{\rho}(r) - \tilde{\rho}(0)}{r} = \tilde{\rho}'(0), \end{aligned} \quad (2.22)$$

and by (2.20) and (2.22), $\tilde{\rho}'(0) = -Z\tilde{\rho}(0)$. This proves (1.14).

Next, define the function $\tilde{\eta}$ by the equations

$$\tilde{\rho}(r) = e^{-Zr}(\tilde{\rho}(0) + \beta r^2 + \tilde{\eta}(r)), \quad (2.23)$$

$$\beta = \frac{1}{3}(\tilde{h}(0) - \frac{Z^2}{2}\tilde{\rho}(0)).$$

Then $\tilde{\eta}(0) = 0$, and due to (1.14), $\tilde{\eta}'(0) = 0$. Together with (1.9) this gives

$$\begin{aligned}\Delta\tilde{\eta}(r) &= \left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\right)\tilde{\eta} \\ &= 2\left[e^{Zr}\tilde{h}(r) - \frac{Z^2}{2}\tilde{\rho}(r)e^{Zr} - 3\beta + 2Z\beta r + Z\tilde{\eta}'(r)\right] \\ &\equiv 2G(r).\end{aligned}\tag{2.24}$$

From the foregoing regularity properties of $\tilde{\rho}$, in particular (1.14) and (2.23), we obtain that $\tilde{\eta}' \in C^0([0, \infty))$. From this, together with the regularity properties of \tilde{h} shown in Section 3, we conclude that $G \in C^0([0, \infty))$ and

$$G(r) \rightarrow \tilde{h}(0) - \frac{Z^2}{2}\tilde{\rho}(0) - 3\beta = 0 \quad \text{as } r \downarrow 0.\tag{2.25}$$

From (2.25) and (2.24) we get that

$$\tilde{\eta}(r) = 2 \int_0^r \frac{1}{t^2} \int_0^t G(s)s^2 ds dt,$$

and

$$\frac{\tilde{\eta}'(r) - \tilde{\eta}'(0)}{r} = \frac{2}{r^3} \int_0^r G(s)s^2 ds = \frac{2}{3} \frac{1}{\text{Vol}_{\mathbb{R}^3}(B(0, r))} \int_{B(0, r)} G(|x|) d^3x,$$

so that

$$\eta''(0) = \lim_{r \downarrow 0} \frac{\eta'(r) - \eta'(0)}{r} = \frac{2}{3} G(0) = 0.\tag{2.26}$$

Then by (2.23) $\tilde{\rho}''(0)$ exists, and

$$\tilde{\rho}''(0) = Z^2\tilde{\rho}(0) + 2\beta = \frac{2}{3}(\tilde{h}(0) + Z^2\tilde{\rho}(0)).$$

This verifies (1.13).

Furthermore, by (2.24),

$$\Delta\tilde{\eta}(r) = \tilde{\eta}''(r) + \frac{2}{r}\tilde{\eta}'(r) = 2G(r)$$

and so

$$\tilde{\eta}''(r) = 2G(r) - \frac{2}{r}\tilde{\eta}'(r) = 2G(r) - 2\left(\frac{\tilde{\eta}'(r) - \tilde{\eta}'(0)}{r}\right)$$

since $\tilde{\eta}'(0) = 0$. This implies, by (2.26),

$$\lim_{r \downarrow 0} \tilde{\eta}''(r) = 2\left(\lim_{r \downarrow 0} G(r) - \lim_{r \downarrow 0} \left(\frac{\tilde{\eta}'(r) - \tilde{\eta}'(0)}{r}\right)\right) = \tilde{\eta}''(0) = 0,$$

so that due to (2.23) $\tilde{\rho}''(r)$ is continuous at $r = 0$. Hence formula (1.13) follows from (2.23) and $\tilde{\eta}''(0) = 0$. This finishes the proof of Theorem 1.11. \square

3. REGULARITY OF h AND \tilde{h}

In this section we prove the statements in Theorem 1.11 on the regularity of the functions h and \tilde{h} . More precisely, we prove the following:

Proposition 3.1. *Let ψ satisfy (1.3) and let h be as in (2.8):*

$$\begin{aligned} h(x) = & \int_{\mathbb{R}^{3(N-1)}} |\nabla \psi|^2 dx_2 \cdots dx_N \\ & - \sum_{j=2}^N \int_{\mathbb{R}^{3(N-1)}} \frac{Z}{|x_j|} \psi^2 dx_2 \cdots dx_N \\ & + \sum_{1 \leq j < k \leq N} \int_{\mathbb{R}^{3(N-1)}} \frac{1}{|x_j - x_k|} \psi^2 dx_2 \cdots dx_N, \end{aligned} \quad (3.1)$$

and \tilde{h} as in (2.14):

$$\tilde{h}(r) = \int_{\mathbb{S}^2} h(r\omega) d\omega.$$

Then $h \in C_{\text{loc}}^\alpha(\mathbb{R}^3 \setminus \{0\})$ and $\tilde{h} \in C^0([0, \infty)) \cap C_{\text{loc}}^\alpha((0, \infty))$ for all $\alpha \in (0, 1)$.

Remark 3.2. From the proof of Proposition 3.1 follows the continuity of the function t_1 in Remark 1.15.

Proof. For convenience, we shall often write $\int \equiv \int_{\mathbb{R}^{3(N-1)}}$. Let

$$\begin{aligned} J_1(x) &= \int |\nabla \psi|^2 dx_2 \cdots dx_N, \\ J_2(x) &= \sum_{j=2}^N \int \frac{Z}{|x_j|} \psi^2 dx_2 \cdots dx_N, \\ J_3(x) &= \sum_{1 \leq j < k \leq N} \int \frac{1}{|x_j - x_k|} \psi^2 dx_2 \cdots dx_N. \end{aligned} \quad (3.2)$$

For the proof of the regularity of the functions J_1, J_2, J_3 we shall make use of the following lemmas. The proof of the first lemma is trivial, using $|(x_1, x_2, \dots, x_N)| \geq |(x_2, \dots, x_N)|$.

Lemma 3.3. *Let $\alpha \in (0, 1)$ and $x_0 \in \mathbb{R}^3$. Assume that the real function $G = G(x_1, \dots, x_N)$ satisfies: For all $R > 0$ there exists constants C, γ such that*

$$\begin{aligned} &\sup_{x, y \in B(x_0, R)} \frac{|G(x, x_2, \dots, x_N) - G(y, x_2, \dots, x_N)|}{|x - y|^\alpha} \leq \\ &C \exp(-\gamma|(x_0, x_2, \dots, x_N)|) \quad \text{for all } (x_0, x_2, \dots, x_N) \in \mathbb{R}^{3N}. \end{aligned} \quad (3.3)$$

Then the function

$$\eta(x) \equiv \int_{\mathbb{R}^{3(N-1)}} G(x, x_2, \dots, x_N) dx_2 \cdots dx_N$$

is in $C_{loc}^\alpha(\mathbb{R}^3)$.

We next prove the following lemma.

Lemma 3.4. *Let $\alpha \in (0, 1)$. Assume that the real valued function $K = K(x_1, \dots, x_N)$ satisfies (3.3) and that there exists constants C, γ such that*

$$\begin{aligned} & |K(x_1, \dots, x_N)| \\ & \leq C \exp(-\gamma|(x_1, \dots, x_N)|) \text{ for all } (x_1, \dots, x_N) \in \mathbb{R}^{3N}. \end{aligned} \quad (3.4)$$

Then:

(a)

For all $j, k \in \{1, \dots, N\}, j \neq k$, the function

$$\zeta(x_1) \equiv \int_{\mathbb{R}^{3(N-1)}} \frac{1}{|x_j - x_k|} K(x_1, \dots, x_N) dx_2 \cdots dx_N$$

is in $C_{loc}^\alpha(\mathbb{R}^3)$.

(b)

For $j \geq 2$ the function

$$\mu(x_1) \equiv \int_{\mathbb{R}^{3(N-1)}} \frac{1}{|x_j|} K(x_1, \dots, x_N) dx_2 \cdots dx_N$$

is in $C_{loc}^\alpha(\mathbb{R}^3)$.

Proof. Assume first that $j \neq 1 \neq k$. Let $x, y \in B(x_0, R)$, then by (3.3),

$$\begin{aligned} & \frac{|\zeta(x) - \zeta(y)|}{|x - y|^\alpha} \leq \\ & \int \frac{1}{|x_j - x_k|} \frac{|K(x, x_2, \dots, x_N) - K(y, x_2, \dots, x_N)|}{|x - y|^\alpha} dx_2 \cdots dx_N \\ & \leq C \int \frac{1}{|x_j - x_k|} \exp(-\gamma|(x_0, x_2, \dots, x_N)|) dx_2 \cdots dx_N. \end{aligned}$$

By equivalence of norms in \mathbb{R}^{3N} there is a constant c_0 such that

$$\begin{aligned} & \frac{|\zeta(x) - \zeta(y)|}{|x - y|^\alpha} \leq C \left(\prod_{l=2, l \neq j, k}^N \int_{\mathbb{R}^3} \exp(-\gamma c_0 |x_l|) dx_l \right) \times \\ & \times \int_{\mathbb{R}^6} \frac{1}{|x_j - x_k|} \exp(-\gamma c_0 (|x_j| + |x_k|)) dx_j dx_k \leq C, \quad x, y \in B(x_0, R). \end{aligned}$$

The last inequality is an application of the following inequality (with $n = 3, \lambda = 1, p = r = 6/5$): (see Lieb and Loss [10, Theorem 4.3])

Hardy-Littlewood-Sobolev Inequality: Let $p, r > 1$ and $0 < \lambda < n$ with $1/p + \lambda/n + 1/r = 2$. Let $f \in L^p(\mathbb{R}^n)$ and $h \in L^r(\mathbb{R}^n)$. Then there exists a sharp constant $C(n, \lambda, p)$, independent of f and h , such that

$$\left| \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f(x) |x - y|^{-\lambda} h(y) dx dy \right| \leq C(n, \lambda, p) \|f\|_p \|h\|_r.$$

This proves Lemma 3.4 (a) when $j \neq 1 \neq k$.

Assume now that $j = 1$. We assume without loss that $k = 2$. Then, with $x_1, \bar{x}_1 \in B(x_0, R)$,

$$\begin{aligned} \frac{|\zeta(x_1) - \zeta(\bar{x}_1)|}{|x_1 - \bar{x}_1|^\alpha} &\leq \\ &\int \frac{1}{|x_1 - x_2|} \frac{|K(x_1, x_2, \dots, x_N) - K(\bar{x}_1, x_2, \dots, x_N)|}{|x_1 - \bar{x}_1|^\alpha} dx_2 \cdots dx_N \\ &+ \int \left| \frac{1}{|x_1 - x_2|} - \frac{1}{|\bar{x}_1 - x_2|} \right| |x_1 - \bar{x}_1|^{-\alpha} |K(\bar{x}_1, x_2, \dots, x_N)| dx_2 \cdots dx_N \\ &\equiv (A) + (B). \end{aligned}$$

For (A), using (3.3) and equivalence of norms in \mathbb{R}^{3N} , we get

$$\begin{aligned} (A) &\leq C \int \frac{1}{|x_1 - x_2|} \exp(-\gamma c_0(|x_0| + |x_2| + \cdots + |x_N|)) dx_2 \cdots dx_N \\ &\leq C \int_{\mathbb{R}^3} \frac{1}{|x_1 - x_2|} \exp(-\gamma c_0|x_2|) dx_2 \leq C(x_0, R). \end{aligned}$$

As for (B), we apply the following inequality; for the convenience of the reader, we give the proof (borrowed from Lieb and Loss [10, (3) p. 225]).

For $\alpha \in (0, 1)$:

$$\begin{aligned} \left| \frac{1}{|x - z|} - \frac{1}{|y - z|} \right| |x - y|^{-\alpha} &\leq \\ |x - z|^{-1-\alpha} + |y - z|^{-1-\alpha} &\quad \text{for all } x, y, z \in \mathbb{R}^3. \end{aligned} \tag{3.5}$$

Proof of (3.5). By Hölder's inequality we have, for $b > 1$, $\alpha \in (0, 1)$,

$$1 - b^{-1} = \int_1^b t^{-2} dt \leq \left(\int_1^b dt \right)^\alpha \left(\int_1^\infty t^{-2/(1-\alpha)} dt \right)^{1-\alpha} \leq (b-1)^\alpha.$$

Substituting b/a for b , with $a > 0$, this gives

$$|b^{-1} - a^{-1}| \leq |b - a|^\alpha \max\{a^{-1-\alpha}, b^{-1-\alpha}\}.$$

So, for $x, y, z \in \mathbb{R}^3$, using $\max\{s, t\} \leq s + t$ and the triangle inequality in \mathbb{R}^3 , we have

$$||x - z|^{-1} - |y - z|^{-1}| \leq |x - y|^\alpha \{ |x - z|^{-1-\alpha} + |y - z|^{-1-\alpha} \}.$$

□

In this way, by (3.4) and equivalence of norms in \mathbb{R}^{3N} ,

$$\begin{aligned} (\text{B}) &\leq \int \left(\frac{|K(\bar{x}_1, x_2, \dots, x_N)|}{|x_1 - x_2|^{1+\alpha}} + \frac{|K(\bar{x}_1, x_2, \dots, x_N)|}{|\bar{x}_1 - x_2|^{1+\alpha}} \right) dx_2 \cdots dx_N \\ &\leq C \prod_{j=3}^N \int_{\mathbb{R}^3} \exp(-\gamma c_0 |x_j|) dx_j \\ &\quad \times \int_{\mathbb{R}^3} \left(\frac{1}{|\bar{x}_1 - x_2|^{1+\alpha}} + \frac{1}{|x_1 - x_2|^{1+\alpha}} \right) \exp(-\gamma c_0 |x_2|) dx_2 \\ &\leq C(x_0, R), \end{aligned}$$

since $x_1, \bar{x}_1 \in B(x_0, R)$. This finishes the proof of Lemma 3.4 (a).

The proof of (b) is similar to that of (a) so we omit the details. \square

The proof of the following fact is straightforward:

There exist constants $C = C(\gamma, R)$ and $\tilde{\gamma} = \tilde{\gamma}(\gamma)$ such that

$$\exp(-\gamma|(x, \dots, x_N)|) \leq C \exp(-\tilde{\gamma}|(x_0, \dots, x_N)|) \quad (3.6)$$

for all $x \in B(x_0, R)$.

Using this and Lemma 3.3, 3.4, we shall prove the following lemma on the regularity of the functions J_1, J_2 and J_3 from (3.2).

Lemma 3.5. *Let J_1, J_2 and J_3 be as in (3.2). Then*

- (i) $J_2, J_3 \in C_{\text{loc}}^\alpha(\mathbb{R}^3)$ for all $\alpha \in (0, 1)$.
- (ii) $J_1 \in C_{\text{loc}}^\alpha(\mathbb{R}^3 \setminus \{0\})$ for all $\alpha \in (0, 1)$.

Herefrom follow the regularity properties of the function h stated in Proposition 3.1.

Proof of Lemma 3.5 (i).

Firstly, by Theorem 1.2 and Remark 1.8,

$$|\psi(\mathbf{x})|, |\nabla\psi(\mathbf{x})| \leq C \exp(-\gamma|\mathbf{x}|), \quad \mathbf{x} \in \mathbb{R}^{3N}, \quad (3.7)$$

which gives (3.4) for $K = \psi^2$.

Next we verify that for $G = \psi^2$, (3.3) is fulfilled. Then Lemma 3.4 can be applied with $K = \psi^2$, and the Hölder-continuity of J_2 and J_3 follows.

Given $x_0 \in \mathbb{R}^3, R > 0, \alpha \in (0, 1)$, and $x, y \in B(x_0, R)$. Using that (see e. g. Malý and Ziemer [11, Theorem 1.41]) (here, $(x, x_2, \dots, x_N) = (x, x'), x' \in \mathbb{R}^{3(N-1)}$)

$$\begin{aligned} \psi^2(x, x') - \psi^2(y, x') &= \int_0^1 \frac{\partial}{\partial s} [\psi^2(sx + (1-s)y, x')] ds \\ &= \int_0^1 [\nabla_1(\psi^2)(sx + (1-s)y, x')] \cdot (x - y) ds \end{aligned} \quad (3.8)$$

and that $sx + (1 - s)y \in B(x_0, R)$ for all $s \in [0, 1]$ we get, with (3.7) and (3.6),

$$\begin{aligned} & \frac{|\psi^2(x, x') - \psi^2(y, x')|}{|x - y|^\alpha} \\ & \leq 2|x - y|^{1-\alpha} \int_0^1 |\nabla_1 \psi(sx + (1 - s)y, x')| \cdot |\psi(sx + (1 - s)y, x')| ds \\ & \leq 2(2R)^{1-\alpha} \int_0^1 C \exp(-2\gamma|(sx + (1 - s)y, x')|) ds \\ & \leq C \exp(-\tilde{\gamma}|(x_0, \dots, x_N)|), \end{aligned} \quad (3.9)$$

so (3.3) follows for $\alpha \in (0, 1)$.

This proves (i) of Lemma 3.5.

To prove (ii), we write ψ as in the proof of Theorem 1.2: $\psi = e^{F-F_1}\psi_1$, with F and F_1 as in (1.6) and (2.1). Then

$$\begin{aligned} J_1(x) &= \int |\nabla \psi|^2 dx' = \int |\nabla F|^2 \psi^2 dx' + \int |\nabla F_1|^2 \psi^2 dx' \\ &\quad - 2 \int (\nabla F \cdot \nabla F_1) \psi^2 dx' + \int e^{2(F-F_1)} |\nabla \psi_1|^2 dx' \\ &\quad + 2 \int (\nabla F \cdot \nabla \psi_1) e^{2(F-F_1)} \psi_1 dx' - 2 \int (\nabla F_1 \cdot \nabla \psi_1) e^{2(F-F_1)} \psi_1 dx' \\ &\equiv I_1(x) + I_2(x) + I_3(x) + I_4(x) + I_5(x) + I_6(x). \end{aligned} \quad (3.10)$$

Using the idea from (3.8) twice (on $|\nabla F_1|^2$ and ψ^2 , respectively), the estimates (2.3), (3.7), (3.9), and (3.6), we have, with $x_0 \in \mathbb{R}^3, R > 0, \alpha \in (0, 1)$, and $x, y \in B(x_0, R)$:

$$\begin{aligned} & \frac{||\nabla F_1|^2 \psi^2(x, x') - |\nabla F_1|^2 \psi^2(y, x')||}{|x - y|^\alpha} \leq \\ & \quad \frac{||\nabla F_1(x, x')|^2 - |\nabla F_1(y, x')|^2||}{|x - y|^\alpha} |\psi(x, x')|^2 \\ & \quad + |\nabla F_1(y, x')|^2 \frac{|\psi^2(x, x') - \psi^2(y, x')|}{|x - y|^\alpha} \\ & \leq C |x - y|^{1-\alpha} \|\nabla(|\nabla F_1|^2)\|_\infty \exp(-2\gamma|(x, x_2, \dots, x_N)|) \\ & \quad + 2\tilde{C} |x - y|^{1-\alpha} \|\nabla F_1\|^2_\infty \exp(-\tilde{\gamma}|(x_0, \dots, x_N)|) \\ & \leq \bar{C} \exp(-\bar{\gamma}|(x_0, \dots, x_N)|). \end{aligned}$$

By Lemma 3.3, with $G = |\nabla F_1|^2 \psi^2(x_1, \dots, x_N)$, this implies that $I_2 \in C_{\text{loc}}^\alpha(\mathbb{R}^3)$.

Using the same ingredients, writing $\nabla \psi_1 = \nabla(e^{F_1-F}\psi)$, gives (3.3) and (3.4) with

$$G = K = e^{2(F-F_1)} |\nabla \psi_1|^2$$

and

$$G = K = (\nabla F_1 \cdot \nabla \psi_1) e^{2(F-F_1)} \psi_1,$$

and so by Lemma 3.3, $I_4, I_6 \in C_{\text{loc}}^\alpha(\mathbb{R}^3)$.

The remaining terms are those involving the function F , namely I_1 , I_3 and I_5 .

Note that

$$\begin{aligned} \nabla F(x_1, \dots, x_N) = & -\frac{Z}{2} \left(\frac{x_1}{|x_1|}, \dots, \frac{x_N}{|x_N|} \right) \\ & + \frac{1}{4} \left(\sum_{k=2}^N \frac{x_1 - x_k}{|x_1 - x_k|}, \dots, \sum_{k=1, k \neq j}^N \frac{x_j - x_k}{|x_j - x_k|}, \dots, \sum_{k=1}^{N-1} \frac{x_N - x_k}{|x_N - x_k|} \right) \end{aligned} \quad (3.11)$$

and so

$$\begin{aligned} |\nabla F(x_1, \dots, x_N)|^2 = & \frac{NZ^2}{4} - \frac{Z}{8} \sum_{j,k=1, k \neq j}^N \frac{x_j}{|x_j|} \cdot \frac{x_j - x_k}{|x_j - x_k|} \\ & + \frac{1}{16} \sum_{j,k,l=1, k \neq j, l \neq j}^N \frac{x_j - x_k}{|x_j - x_k|} \cdot \frac{x_j - x_l}{|x_j - x_l|}. \end{aligned}$$

In this way,

$$\begin{aligned} I_1(x_1) = & \frac{NZ^2}{4} \int \psi^2 dx_2 \cdots dx_N \\ & - \frac{Z}{8} \sum_{j,k=1, k \neq j}^N \int \frac{x_j}{|x_j|} \cdot \frac{x_j - x_k}{|x_j - x_k|} \psi^2 dx_2 \cdots dx_N \\ & + \frac{1}{16} \sum_{j,k,l=1, k \neq j, l \neq j}^N \frac{x_j - x_k}{|x_j - x_k|} \cdot \frac{x_j - x_l}{|x_j - x_l|} \psi^2 dx_2 \cdots dx_N \\ = & \frac{NZ^2}{4} \rho(x_1) - \frac{Z}{8} \sum_{j,k=1, k \neq j}^N \kappa_{j,k}(x_1) + \frac{1}{16} \sum_{j,k,l=1, k \neq j, l \neq j}^N \nu_{j,k,l}(x_1). \end{aligned} \quad (3.12)$$

Note that $\nu_{j,k,l} = \nu_{j,l,k}$.

Using the ideas above, Lemma 3.3 implies that the following functions from (3.12) (with the mentioned choices of G satisfying (3.3)) are

all in $C_{\text{loc}}^\alpha(\mathbb{R}^3)$:

$$\begin{aligned}\rho : \quad G &= \psi^2, \\ \kappa_{j,k}, \quad j, k \neq 1, j \neq k : \quad G &= \frac{x_j}{|x_j|} \cdot \frac{x_j - x_k}{|x_j - x_k|} \psi^2, \\ \nu_{j,k,k}, j \neq k : \quad G &= \frac{x_j - x_k}{|x_j - x_k|} \cdot \frac{x_j - x_k}{|x_j - x_k|} \psi^2 = \psi^2, \\ \nu_{j,k,l}, \quad j, k, l \neq 1, l \neq j \neq k : \quad G &= \frac{x_j - x_k}{|x_j - x_k|} \cdot \frac{x_j - x_l}{|x_j - x_l|} \psi^2.\end{aligned}$$

Likewise, Lemma 3.4 implies (with the mentioned choices of $G = K$ satisfying (3.3) and (3.4)) that the following functions from (3.12) are all in $C_{\text{loc}}^\alpha(\mathbb{R}^3)$:

$$\begin{aligned}\kappa_{j,1}, \quad j \neq 1 : \quad G = K &= \frac{x_j \cdot (x_j - x_1)}{|x_j|} \psi^2, \\ \nu_{j,1,l}, \quad j, l \neq 1, j \neq l : \quad G = K &= \frac{(x_j - x_1) \cdot (x_j - x_l)}{|x_j - x_l|} \psi^2,\end{aligned}$$

From the decomposition of I_1 in (3.12) we are left with

$$\kappa_{1,k}(x_1) = \int \frac{x_1}{|x_1|} \cdot \frac{x_1 - x_k}{|x_1 - x_k|} \psi^2 dx' \quad , \quad k = 2, \dots, N, \quad (3.13)$$

and

$$\nu_{1,k,l}(x_1) = \int \frac{x_1 - x_k}{|x_1 - x_k|} \cdot \frac{x_1 - x_l}{|x_1 - x_l|} \psi^2 dx' \quad , \quad k, l \in \{2, \dots, N\}, k \neq l. \quad (3.14)$$

Note that

$$\begin{aligned}\int \frac{x_1}{|x_1|} \cdot \frac{x_1 - x_k}{|x_1 - x_k|} \psi^2 dx_2 \cdots dx_N \\ = \frac{1}{|x_1|} \int \frac{1}{|x_1 - x_k|} (x_1 \cdot (x_1 - x_k) \psi^2) dx_2 \cdots dx_N.\end{aligned}$$

The function $1/|x_1|$ is smooth for $x_1 \neq 0$ and therefore in $C_{\text{loc}}^\alpha(\mathbb{R}^3 \setminus \{0\})$. The function $x_1 \cdot (x_1 - x_k) \psi^2$ satisfies (3.3) and (3.4) (by the same ideas as above), so Lemma 3.4 (a) implies that the function

$$\int \frac{1}{|x_1 - x_k|} (x_1 \cdot (x_1 - x_k) \psi^2) dx_2 \cdots dx_N$$

is in $C_{\text{loc}}^\alpha(\mathbb{R}^3)$. The functions in (3.13) are therefore in $C_{\text{loc}}^\alpha(\mathbb{R}^3 \setminus \{0\})$.

As for the functions in (3.14), these are all in $C_{\text{loc}}^\alpha(\mathbb{R}^3)$, which can be seen by applying the previous ideas, in particular Lemma 3.5, (3.6), (3.7) and (3.9).

This proves that $I_1 \in C_{\text{loc}}^\alpha(\mathbb{R}^3 \setminus \{0\})$.

As for I_3 (see (3.10) and (3.11)), with $\nabla = (\nabla_1, \dots, \nabla_N)$,

$$\begin{aligned} I_3(x) &= Z \sum_{j=1}^N \int \left(\frac{x_j}{|x_j|} \cdot \nabla_j F_1 \right) \psi^2 dx_2 \cdots dx_N \\ &\quad - \frac{1}{2} \sum_{j,k=1, j \neq k}^N \int \left(\frac{x_j - x_k}{|x_j - x_k|} \cdot \nabla_j F_1 \right) \psi^2 dx_2 \cdots dx_N. \end{aligned} \quad (3.15)$$

The terms in the first sum with $j \neq 1$ are in $C_{\text{loc}}^\alpha(\mathbb{R}^3)$, due to Lemma 3.4 (b), with $G = K = (x_j \cdot \nabla_j F_1) \psi^2$ satisfying (3.3) and (3.4). (To see this, use the previous ideas; to apply the idea from (3.8) to $\nabla_j F_1$ we use that F_1 is smooth). The terms in the second sum in (3.15) are all in $C_{\text{loc}}^\alpha(\mathbb{R}^3)$, due to Lemma 3.4 (a), applied with $G = K = ((x_j - x_k) \cdot \nabla_j F_1) \psi^2$. The term with $j = 1$ is in $C_{\text{loc}}^\alpha(\mathbb{R}^3 \setminus \{0\})$. This can be seen by following the ideas in the proof of the regularity properties of the function in (3.13), now using Lemma 3.3 with $G = (x_1 \cdot \nabla_1 F_1) \psi^2$.

The statements and proofs are similar for

$$\begin{aligned} I_5(x) &= -Z \sum_{j=1}^N \int \left(\frac{x_j}{|x_j|} \cdot \nabla_j \psi_1 \right) e^{2(F-F_1)} \psi_1 dx_2 \cdots dx_N \\ &\quad + \frac{1}{2} \sum_{j,k=1, j \neq k}^N \int \left(\frac{x_j - x_k}{|x_j - x_k|} \cdot \nabla_j \psi_1 \right) e^{2(F-F_1)} \psi_1 dx_2 \cdots dx_N. \end{aligned} \quad (3.16)$$

That is, the functions in the first sum in (3.16) with $j \geq 2$ and those in the second sum are all in $C_{\text{loc}}^\alpha(\mathbb{R}^3)$, whereas the function in the first sum with $j = 1$ is only in $C_{\text{loc}}^\alpha(\mathbb{R}^3 \setminus \{0\})$. To prove this we use the inequality (with $\mathbf{x} = (x_1, \dots, x_N)$):

$$|\psi_1|_{C^{1,\alpha}(B(\mathbf{x}, R/2))} \leq C \sup_{y \in (B(\mathbf{x}, R))} |\psi_1(y)| \leq C \exp(-\gamma |(x_1, \dots, x_N)|).$$

This inequality follows from (2.3), (2.5) and (3.7) (remember that $\psi_1 = e^{F_1 - F} \psi$).

This proves that $I_5 \in C_{\text{loc}}^\alpha(\mathbb{R}^3 \setminus \{0\})$, and so finishes the proof that $J_1 \in C_{\text{loc}}^\alpha(\mathbb{R}^3 \setminus \{0\})$. (See (3.10)). This proves (ii) and therefore Lemma 3.5. \square

That $\tilde{h} \in C_{\text{loc}}^\alpha((0, \infty))$ is a consequence of the foregoing and of the following proposition:

Proposition 3.6. *Assume $f \in C_{\text{loc}}^\alpha(\mathbb{R}^3 \setminus \{0\})$, $\alpha \in (0, 1)$. Then $\tilde{f} \in C_{\text{loc}}^\alpha((0, \infty))$, where*

$$\tilde{f}(r) = \int_{\mathbb{S}^2} f(r\omega) d\omega.$$

Proof. Let $r \in (0, \infty)$. For all $x_0 \in A = \{x \in \mathbb{R}^3 \mid |x| = r\}$, choose $R = R(x_0)$ and $C = C(x_0)$ such that

$$\sup_{x,y \in B(x_0, R(x_0))} \frac{|f(x) - f(y)|}{|x - y|^\alpha} \leq C(x_0). \quad (3.17)$$

This is possible, since $f \in C_{\text{loc}}^\alpha(\mathbb{R}^3 \setminus \{0\})$. Then

$$A \subset \bigcup_{x_0 \in A} B(x_0, R(x_0)).$$

Using compactness of A , choose $x_1, \dots, x_m \in A$ such that

$$A \subset \bigcup_{j=1}^m B(x_j, R(x_j)).$$

Choose $\epsilon \in (0, r)$ such that

$$\{y \in \mathbb{R}^3 \mid r - \epsilon < |y| < r + \epsilon\} \subset \bigcup_{j=1}^m B(x_j, R(x_j)).$$

Then, for all $s, t \in (r - \epsilon, r + \epsilon)$ and all $\omega \in \mathbb{S}^2$ there exists $j \in \{1, \dots, m\}$ such that $s\omega, t\omega \in B(x_j, R(x_j))$ and therefore by (3.17),

$$\frac{|f(s\omega) - f(t\omega)|}{|s - t|^\alpha} = \frac{|f(s\omega) - f(t\omega)|}{|s\omega - t\omega|^\alpha} \leq C(x_j).$$

So with $C = \max\{C(x_1), \dots, C(x_m)\}$,

$$\frac{|f(s\omega) - f(t\omega)|}{|s - t|^\alpha} \leq C, \text{ for all } s, t \in (r - \epsilon, r + \epsilon) \text{ and all } \omega \in \mathbb{S}^2.$$

This implies that

$$\begin{aligned} \frac{|\tilde{f}(s) - \tilde{f}(t)|}{|s - t|^\alpha} &= \frac{\left| \int_{\mathbb{S}^2} (f(s\omega) - f(t\omega)) d\omega \right|}{|s - t|^\alpha} \\ &\leq \int_{\mathbb{S}^2} \frac{|f(s\omega) - f(t\omega)|}{|s\omega - t\omega|^\alpha} d\omega \leq C, \quad \text{for all } s, t \in (r - \epsilon, r + \epsilon). \end{aligned}$$

This proves that $\tilde{f} \in C_{\text{loc}}^\alpha((0, \infty))$. □

To prove that $\tilde{h} \in C^0([0, \infty))$, we apply the following:

Proposition 3.7. *Assume $f \in C_{\text{loc}}^\alpha(\mathbb{R}^3)$. Then $\tilde{f} \in C^0([0, \infty))$, where*

$$\tilde{f}(r) = \int_{\mathbb{S}^2} f(r\omega) d\omega.$$

Proof. The function f is continuous in \mathbb{R}^3 , since it is in $C_{\text{loc}}^\alpha(\mathbb{R}^3)$. Let $r \in [0, \infty)$. Then

$$\lim_{s \rightarrow r} f(s\omega) = f(r\omega) \quad \text{for all } \omega \in \mathbb{S}^2.$$

Using the supremum of f on a sufficiently large compact set in \mathbb{R}^3 as a dominant, Lebesgue's Dominated Convergence Theorem gives us that

$$\lim_{s \rightarrow r} \int_{\mathbb{S}^2} f(s\omega) d\omega = \int_{\mathbb{S}^2} f(r\omega) d\omega.$$

Therefore $f \in C^0([0, \infty))$. \square

Recall the proof of the fact that $h \in C_{\text{loc}}^\alpha(\mathbb{R}^3 \setminus \{0\})$. In fact, the only terms in the decomposition of h (see (3.1), (3.2), (3.10), and (3.11)) that are only in $C_{\text{loc}}^\alpha(\mathbb{R}^3 \setminus \{0\})$ and not in $C_{\text{loc}}^\alpha(\mathbb{R}^3)$ are the functions

$$\begin{aligned} & \int \frac{x_1}{|x_1|} \cdot \frac{x_1 - x_k}{|x_1 - x_k|} \psi^2 dx_2 \cdots dx_N , \quad k = 2, \dots, N, \\ & \int \left(\frac{x_1}{|x_1|} \cdot \nabla_1 F_1 \right) \psi^2 dx_2 \cdots dx_N, \\ & \int \left(\frac{x_1}{|x_1|} \cdot \nabla_1 \psi_1 \right) e^{2(F - F_1)} \psi_1 dx_2 \cdots dx_N. \end{aligned} \quad (3.18)$$

Comparing (3.10), (3.13), (3.15) and (3.16), it can be seen that all the terms in (3.18) stem from the function J_1 , namely from I_1 , I_3 , and I_5 .

All other terms in the decomposition of h are in $C_{\text{loc}}^\alpha(\mathbb{R}^3)$. When integrating them over \mathbb{S}^2 , we get something continuous in $[0, \infty)$, according to Proposition 3.7 above.

For the terms in (3.18) we note that they are all of the form

$$\int \frac{x_1}{|x_1|} \cdot \mathbf{K}(x_1, x') dx' = \frac{x_1}{|x_1|} \cdot \int \mathbf{K}(x_1, x') dx'. \quad (3.19)$$

In each case, we have

$$\mathbf{L}(x_1) = (L_1(x_1), L_2(x_1), L_3(x_1)) = \int \mathbf{K}(x_1, x') dx', \quad L_j \in C_{\text{loc}}^\alpha(\mathbb{R}^3). \quad (3.20)$$

To see this, apply Lemma 3.3 to each of the coordinate functions L_j , $j = 1, 2, 3$. The integrands are easily seen to satisfy (3.3) in each case, by the previous ideas. To get continuity in $[0, \infty)$ of the functions in (3.18) we use (3.19) and (3.20), and the following lemma:

Proposition 3.8. *Assume $\mathbf{f} = (f_1, f_2, f_3)$, $f_j \in C_{\text{loc}}^\alpha(\mathbb{R}^3)$. Then $\bar{f} \in C^0([0, \infty))$, where*

$$\bar{f}(r) = \int_{\mathbb{S}^2} (\omega \cdot \mathbf{f}(r\omega)) d\omega.$$

Proof. The same as for Proposition 3.7, noting that for all $r \in [0, \infty)$ and fixed $\omega \in \mathbb{S}^2$:

$$\lim_{s \rightarrow r} \omega \cdot \mathbf{f}(s\omega) = \omega \cdot \mathbf{f}(r\omega).$$

\square

This holds even in the case $r = 0$, for which

$$\lim_{s \downarrow 0} \int_{\mathbb{S}^2} \omega \cdot \mathbf{f}(s\omega) d\omega = \int_{\mathbb{S}^2} \omega \cdot \mathbf{f}(0) d\omega = 0.$$

This proves that the functions in (3.18) are in $C^0([0, \infty))$. Therefore $\tilde{h} \in C^0([0, \infty))$, which finishes the proof of Proposition 3.1. \square

Acknowledgement: The authors wish to thank G. Friesecke and S. Fournais for stimulating discussions.

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